Slip Energy Barriers in Aluminum and Implications for Ductile versus Brittle Behavior

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We conisder the brittle versus ductile behavior of aluminum in the framework of the Peierls-model analysis of dislocation emission from a crack tip. To this end, we perform first-principles quantum mechanical calculations for the unstable stacking energy γ_{us} of aluminum along the Shockley partial slip route. Our calculations are based on density functional theory and the local density approximation and include full atomic and volume relaxation. We find that in aluminum $\gamma_{us} = 0.224$ J/m^2. Within the Peierls-model analysis, this value would predict a brittle solid which poses an interesting problem since aluminum is typically considered ductile. The resolution may be given by one of three possibilites: (a) Aluminum is indeed brittle at zero temperature, and becomes ductile at a finite temperature due to motion of pre-existing dislocations which relax the stress concentration at the crack tip. (b) Dislocation emission at the crack tip is itself a thermally activated process. (c) Aluminum is actually ductile at all temperatures and the theoretical model employed needs to be significantly improved in order to resolve the apparent contradiction.

I. INTRODUCTION

Understanding the ductile versus brittle (D/B) response of materials is both scientifically challenging and technologically important. The D/B response of most metals is usually established by experimental methods. A theoretical framework that can describe quantitatively D/B behavior has been pursued for over two decades, beginning with the seminal work of Rice and Thomson (1974). When dealing with complicated high-performance materials, like intermetallic compounds, silicides, etc. the ability to predict the D/B behavior from theoretical considerations becomes even more important, since experimental measurements are not available, or are difficult and time consuming. So far, approximate estimates are available for certain systems, based on atomistic simulations that employ simple interatomic potentials [Cheung (1990); Sun, Rice and Truskinovsky (1991); Beltz and Rice (1992); Sun, Beltz and Rice (1993)]. Using a Peierls type of analysis [Peierls (1940)], Rice and coworkers [Rice (1992); Rice, Beltz and Sun (1992); Sun, Beltz and Rice (1993); Rice and Beltz (1994); Sun and Beltz (1995)] have recently developed simple criteria to characterize the D/B behavior. These criteria use few key parameters related

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to the properties of the solid, namely the unstable stacking energy, the surface energy, the shear modulus and the Burgers vector. Zhou, Carlsson and Thomson (1993, 1994) have also developed similar criteria that involve these parameters, using atomistic studies of model systems. Of these parameters, the one that is not accessible experimentally is the unstable stacking energy γ_{us}, identified by Rice (1992) to be the quantity that controls the emission of straight dislocations from the crack tip under shear loading. The value of γ_{us} is the lowest energy barrier that needs to be surmounted when one half of a crystal slides over the other half in going from one ideal configuration to another equivalent one (the lowest barrier may actually occur between an ideal and a metastable configuration, corresponding to nucleation of partial dislocations). The importance of this quantity within the Peierls model makes it desirable to obtain as accurate estimates as possible for γ_{us} in various materials. Kaxiras and Duesbery (1993) have used first-principles quantum mechanical calculations in the context of density functional theory to obtain the value of the unstable stacking energy for silicon, a prototypical covalent material. Here we performed similar calculations for aluminum, a representative simple metal, and analyze the implications of the results for the D/B behavior of aluminum. Related work on the theoretical strength of aluminum using first-principles quantum mechanical calculations has been reported by Paxton et al. (1991).

The metallic nature of Al and the relatively small energy cost for the slip (compared, for example, to Si) require more attention to computational details. Before embarking on the calculation of γ_{us}, we performed several tests to determine the limitations of our calculations. These tests are described in Section II. Section III discusses our results for γ_{us}. Section IV concludes with some discussion of the implications of our results for the D/B behavior of Al in the context of current theories.

II. FIRST-PRINCIPLES CALCULATIONS FOR ALUMINUM

A. Bulk properties

Our first-principles calculations are based on density functional theory [Hohenberg and Kohn (1964)] in the local density approximation [Kohn and Sham (1965)] (in the following referred to as DFT/LDA). We employ the expression for the exchange and correlation functional proposed by Perdew and Zunger (1981), and a norm-conserving non-local pseudopotential from Bachelet, Haman and Schlüter (1982) to represent the atomic core and eliminate the core electrons of Al. A plane wave basis is used to expand the wave functions of the Kohn-Sham orbitals. Since the physical quantities of interest involve obtaining small energy differences by subtracting large numbers, particular care must be taken to assess the uncertainty in these numbers. There are two sources of errors: The first has to do with computational choices, such as limiting the plane

wave basis to sets with kinetic energy up to a maximum value, and approximating integrals over the Brillouin Zone (BZ) by sums over finite sets of reciprocal space points, referred to as k-points; the other source of error has to do with inherent limitations of the formalism we employ. We attempted to minimize the first type of error by variationally expanding the plane wave basis and by enlarging the sets of k-points used in reciprocal space integrations. The theoretical results are reasonably well converged with respect to these computational choices. In order to provide estimates of how much the converged results differ from true physical values, we compare to the values of quantities that can be measured experimentally, specifically the energy of the intrinsic stacking fault in Al. Any residual difference is the error inherent in the calculations due to fundamental limitations of the formalism. We discuss in the concluding section how the present results may be used to extract useful insight despite their limitations.

As a first test we have calculated the equilibrium lattice constant and the elastic properties of fcc bulk Al. For the equilibrium lattice constant we use a cutoff in the kinetic energy of plane waves equal to 12 Ry (corresponding to 70 plane waves per atom) and a uniform grid of k-points in the BZ produced by dividing each of the three primitive vectors in reciprocal space in intervals of equal size [Monkhorst and Pack (1976)]. We use the notation $b_i/\delta k_i = n_i$ to denote the number of divisions in the primitive reciprocal space vectors ($i = 1, 2, 3$), where b_i is the magnitude of a vector and δk_i is the interval corresponding to a certain choice of n_i. In the case of bulk fcc Al, $b_1 = b_2 = b_3$ and therefore we take $n_1 = n_2 = n_3 = 16$. These cutoffs are adequate for well converged calculations of bulk properties. In order to obtain the equilibrium lattice constant from the computed energy as a function of lattice constant, we fit to the universal binding energy relation proposed by Rose et al. (1984),

$$E(a^*) = E_0 + E_c - E_c(1 + a^*)\exp(-a^*) \tag{1}$$

where E_0, E_c correspond to the minimum energy and the cohesive energy respectively, and the reduced lattice constant a^* is given in terms of the actual lattice constant a as $a^* = (a - a_0)/l$ with a_0 the equlibrium lattice constant and l a parameter setting the length scale. In this expression, E_0, a_0, l are viewed as fitting parameters and E_c is taken from experiment $E_c = 3.39$ eV per atom. To obtain the values of the parameters E_0, a_0, l we calculated the energy at 25 points between $a = 3.6$ and 6.4 Å. We find $a_0 = 3.95$ Å. The experimental lattice constant of Al at room temperature is 4.05 Å. In order to compare our theoretical value of the equlibrium lattice constant (which of course is calculated at zero temperature) to the experimental one at room temperature, we use the experimental thermal expansion coefficient $\alpha = 2.36 \times 10^{-5} K^{-1}$ (Pearson (1958)), to extrapolate between zero and room temperature. This gives a theoretical estimate for the lattice constant at room temperature of 4.02 Å, which is in excellent agreement with experiment. We also calculated the bulk modulus B from the second derivative of the energy with respect to volume, evaluated at the point where the first derivative vanishes. We

obtain $B = 84.8$ GPa compared to the experimental result of 76.93 GPa. This difference of 10 % is typical of DFT/LDA calculations.

In addition to a_0 and B, we have calculated the elastic constants $C_{11} - C_{12}$ and C_{44}, which enter in the expression of the shear modulus $\mu = (C_{11} - C_{12} + 3C_{44})/5$. The elastic constants were obtained by using the stress-strain relations, and inducing appropriate distortions of the unit cell. The amount of the distortion was large enough to produce energy differences that can be calculated accurately, yet small enough so that quadratic fits to the energy are appropriate. Typical distortions were in the range of 5 - 10 %. We have performed these calculations with a higher density of sampling points in the BZ. This was deemed necessary because the calculation of elastic constants involves rather small energy differences. We find that their values are converged for $n_1 = n_2 = n_3 = 20$. The values of the elastic constants and the shear modulus are sensitive to the lattice constant of the crystal. Accordingly, we have performed the calculation at two different lattice constants, the theoretical one at zero temperature ($a_0 = 3.95$ Å), and the experimental one at room temperature ($a'_0 = 4.05$ Å). The results are tabulated in Table I. The agreement with experiment is poor at the the theoretical lattice constant at zero temperature, but becomes reasonable at the room-temperature experimental lattice constant. Our results compare favorably with previous calculations performed at the experimental lattice constant a'_0 by Mehl and Boyer (1991).

B. Intrinsic stacking fault energy

As a final test of the reliability of our approach we have calculated the value of the intrinsic stacking fault γ_{isf} in aluminum, a number that can be determined experimentally. An additional advantage of performing this calculation is that the technical aspects are identical to the calculation of the unstable stacking energy. Specifically, both the intrinsic stacking fault and the unstable stacking energy can be obtained by considering a slab and shearing it in a periodic fashion by a certain distance. This is ilustrated in Fig. 1: in 1(a), a top view of the ABCABC stacking of layers in the fcc lattice is displayed with high symmetry directions identified; in 1(b), a side view is shown, with the slip plane identified. The periodic slab consists of an integer multiple of ABC layers in the [111] direction. In our clalculations we have used slabs with two and three periods (i.e. consisting of 6 and 9 layers in the [111] direction), to check convergence with respect to slab size. For slip of $a_0/\sqrt{6}$ in the [12$\bar{1}$] direction, one obtains the intrinsic stacking fault configuration, i.e. a structure that involves the stacking ABCBCABC, with the stacking fault between the third and fourth layers in the sequence. The unstable stacking energy corresponds to a configuration that is sheared partly from the ideal configuration to the intrinsic stacking fault one by an as yet unspecified amount.

For both the intrinsic stacking fault and the unstable stacking energy, we performed the calculations at the theoretically determined lattice constant. This is an important detail that deserves justification: the structure of defects, such as vacancies, interstitials, stacking faults, grain boundaries, etc. involves relaxation of the atomic coordinates to a fully optimized geometry in which the calculated forces on the ions are vanishingly small. In order for the relaxed configuration to make physical sense, one has to keep the crystal far from the defect at its equilibrium lattice constant. In a supercell calculation, the boundaries of the unit cell represent this "far from the defect" region. This ensures that any atomic relaxation in the neighborhood of the defect is the result of the presence of the defect, rather than externally imposed strain. Thus, defect calculations, including the stacking fault ones, must be performed at the theoretical lattice constant.

In the slab calculations, the three lattice vectors are no longer equivalent. The two planar vectors are actually identical to two primitive fcc lattice vectors, for instance along the [110] and [101] directions, as indicated in Fig. 1(a). The third lattice vector is in the [111] direction, and is a multiple of the repeat distance between A layers in that direction. Because of these differences, care must be taken to perform the calculations at the same level of convergence as the bulk calculation, so that the energy of the intrinsic stacking fault and the unstable stacking can be compared to that of the bulk. Specifically, the number of intervals in each reciprocal space direction must be proportional to the length of the reciprocal lattice vector, or equivalently, inversely proportional to the length of the real-space repeat vector. Moreover, the angles between the various vectors must also be taken into account, so that the volume density of reciprocal points in the calculations remains approximately the same. Since in the fcc lattice the primitive vectors form 60^0 angles, whereas in the slab calculation with one vector along the [111] direction two of the angles are 90^0, an extra factor of $\sin(60^0)$ must be included in figuring out the ratios of divisions along the reciprocal lattice directions. With these considerations, we find that the following relations must hold: $n_1 = n_2 = 3\sqrt{2}n_3$ and $n_1 = n_2 = 9/\sqrt{2}n_3$ for the 6-layer and 9-layer slabs respectively, where the repeat vector in the [111] direction is identified with the index 3. These relationships cannot be satisfied exactly for integer divisions of the reciprocal lattice vectors. Instead, we have used the relations $n_1 = n_2 = 4n_3$ and $n_1 = n_2 = 6n_3$ which satisfy the desired ratios to a good approximation. Convergence tests were performed for both the number of divisions along each reciprocal space direction, as well as the number of plane waves per atom. The results of these tests are shown in Fig. 2.

Although the results for the 6-layer and 9-layer supercells are reasonably close, indicating adequate convergence with respect to supercell size, we have performed an additional test to establish how reliable these numbers are. For this test we used the anisotropic next-nearest-neighbor Ising (ANNNI) model to obtain the energy of the intrinsic stacking fault. Details of this approach can be found in the work of Denteneer and Soler (1991a, 1991b). The calculation

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of the intrinsic stacking fault energy is based on assuming coupling constants between different layers, and obtaining the values of the coupling constants by comparing the energies of various periodic stackings, such as ABC (corresponding to the fcc lattice), AB (corresponding to the hcp lattice) and ABCB. Keeping only the lowest order terms, the first two coupling constants J_1, J_2 are given by

$$J_1 = \frac{1}{4}E(AB) - \frac{1}{6}E(ABC) \tag{2}$$

$$J_2 = \frac{1}{4}E(ABCB) - \frac{1}{6}E(ABC) - \frac{1}{2}J_1 \tag{3}$$

and the intrinsic stacking fault is given by

$$\gamma_{isf} = 4(J_1 + J_2)/A \tag{4}$$

where $A = \sqrt{3}a_0^2/4$ is the area per unit cell on the plane of the fault. The advantage of the approach is that very small unit cells can be used to extract the values of the coupling constants, allowing for more extensive convergence tests. The results for γ_{isf} obtained from the ANNNI model are included in Fig. 2 for comparison to the supercell calculations. Taken together, these results indicate that the value of the instrinsic stacking fault is reasonably well converged with a basis of 70 plane waves per atom (corresponding to a kinetic energy cutoff of 12 Ry), and for a density of BZ sampling points corresponding to 16 divisions along the direction of primitive in-plane vectors. The value obtained from these calculations is

$$\gamma_{isf} = 0.165 \pm 0.015 \text{ J/m}^2 \tag{5}$$

The error bar was estimated by assuming that the contributions from (a) the size of the plane-wave basis, (b) the density of BZ sampling points, and (c) the size of the supercell, are independent, as experience with similar calculations and Fig. 2 indicate. The total error is then obtained as the square root of the sum of squares of the three contributions.

The value of γ_{isf} that we obtained is in excellent agreement with the result of Wright et al. (1992) 0.161 J/m^2, who used a similar method in their calculations (the plane-wave pseudopotential approach). Our value for γ_{isf} is higher than the result of Denteneer and Soler (1991a), 0.126 J/m^2, which was obtained with a different computational method (the Augmented Plane Wave (APW) approach). Experimental measurements range from a low of 0.110 J/m^2 to a high of 0.280 J/m^2, with the most recent result at 0.150 J/m^2 (by Mills and Sadelmann (1989) - see Wright et al. (1992) for additional information). Our calculated value is also in excellent agreement with the experimental value 0.166 J/m^2 quoted by Hirth and Lothe (1982).

III. UNSTABLE STACKING FAULT

The value of the unstable stacking energy γ_{us} was obtained by shearing half of the infinite crystal over the other half and finding the lowest energy barrier that needs to be overcome in order to bring the crystal from one ideal configuration to another equivalent one. The path along which the energy barrier is lowest is in one of the equivalent ¡211¿ crystallographic directions, for instance the $[12\bar{1}]$ direction, shown in Fig. 1. Slip along this direction by

$$b_p = a_0/\sqrt{6} \tag{6}$$

leads to the instrinsic stacking fault configuration, which corresponds to a metastable configuration. The unstable stacking energy configuration corresponds to the saddle point along the path from the equilibrium to the metastable configuration, which should occur near, but not necessarily at, the midpoint. To determine the position of the saddle point we calculated the energy for several displacements along the slip path. We refer to these energies as the generalized stacking fault energy γ_{gsf}. The results are shown in Fig. 3. Our calculations indicate that the saddle point configuration occurs at $0.62b_p$. The value of the energy at the saddle point configuration, before any relaxation is taken into account, is

$$\gamma_{us}^{(u)} = 0.249 \text{ J/m}^2. \tag{7}$$

When both atomic relaxation and volume relaxation are taken into account, this value drops by 0.025 J/m^2. Within the Peierls model framework, volume relaxation is meaningful only in the $[111]$ direction. Our estimate of the relaxed unstable stacking energy in aluminum is

$$\gamma_{us}^{(r)} = 0.224 \text{ J/m}^2. \tag{8}$$

Both atomic relaxation and volume relaxation were calculated using the theoretically determined value for the in-plane lattice constant, i.e. $a_0 = 3.95$ Å, so that spurious contributions from strain in the lattice are avoided, as explained in the previous section. Since the unstable stacking energy was obtained by exactly the same computational parameters as the intrinsic stacking fault energy, we expect that the same error bars as determined in the previous section will apply.

It is useful to express the above results for the unrelaxed and relaxed values of the unstable stacking energy in terms of the dimensionless quantities defined by Sun, Beltz and Rice (1993), that provide estimates of the importance of tension-shear coupling. These quantities are defined as:

$$q = \frac{\gamma_{us}^{(u)}}{2\gamma_s}, \ p = \frac{\Delta_\theta^*}{L}, \tag{9}$$

where γ_s is the energy per unit area of the surface exposed during decohesion, Δ_θ^* is the value of the opening displacement when atomic relaxation is included and corresponding to tensile

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stress $\sigma = 0$ at the unstable stacking configuration, and L is a phenomenological length scale for tension. The values of the various quantities in the above equations as obtained from the present calculations and from previous work by Sun, Beltz and Rice (1993) using the embedded atom method (EAM), are given in Table II. In this comparison, we have used the value of $\gamma_s = 1.10$ J/m^2, from the work of Ferrante and Smith (1979), which was obtained using DFT-LDA calculations. The comparison of the two sets of results in Table II, one from the present first-principles calculations, the other from the empirical EAM calculations, reveals that while the bare quantities $\gamma_s, \gamma_{us}^{(u)}, \gamma_{us}^{(r)}$ differ by factors of 2 to 3 in the two calculations, the dimensionless scaled quantities p, q, L are actually rather close. Apparently, the underestimates of the bare quantities by large factors in the EAM calculations cancel out when the scaled quantities p and q are computed, giving reasonable estimates of the shear to tension coupling.

IV. IMPLICATIONS FOR BRITTLE-DUCTILE BEHAVIOR

Significant progress has been made recently in developing criteria for the D/B behavior by the theoretical analysis of Xu, Argon and Ortiz (1995,1996a,1996b) using the boundary integral method, and the studies by Zhou, Carlsson and Thomson (1993,1994), using a Green's function approach and model atomistic systems. The involved nature of these studies reflects the inherent difficulty in capturing a very complex dynamical phenomenon such as brittleness or ductility, with a few parameters. In the spirit of retaining a simple criterion for the D/B behavior, it is worthwhile to examine the implications of the present results for aluminum. We will consider two different contexts: The first is based on the criteria developed by Rice and coworkers [Rice (1992); Rice, Beltz and Sun (1992); Sun, Beltz and Rice (1993); Rice and Beltz (1994); Sun and Beltz (1995)], the second derives from the atomistic studies of model systems by Zhou et al. (1993,1994).

In the context of the Peierls type analysis of Rice and coworkers, one can obtain the critical loading for dislocation emission at a crack tip G_d, which depends on the value of γ_{us} and the external loading (assumed here to be mode I), as well as the geometry of the dislocation to be emitted. In the case of aluminum, the relevant dislocation is a Shockley partial, and the parameters entering in the geometry are the tilt angle θ between the the slip plane and the extension of the crack, and the angle ϕ between the direction in which the dislocation is emitted and its Burgers vector. These features are illustrated in Fig. 4. For the case of tension-shear coupling, the value of G_d (typically given in terms of γ_s, i.e. the ratio $G_d/2\gamma_s$), is obtained by solving numerically a pair of coupled integral equations as described in detail by Sun, Beltz and Rice (1993). We have performed such calculations for the slip route described earlier, for several crack geometries described by the three vectors $\vec{a}_1, \vec{a}_2, \vec{a}_3$, pointing along the crack propagation

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direction, normal to the crack plane and along the crack line, respectively (see Fig. 4). In these calculations we take the surface energy γ_s to be the same for the (111) and (001) surfaces (which is true to a good approximation), and we use the experimental values for the elastic constants from Hirth and Lothe (1982).

The results of our calculations are shown in Table III. The geometry labeled A, with $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\} = \{[\bar{1}10], [001], [110]\}$, i.e. with a crack on the (001) plane, is interesting in that it produces a ratio $G_d/2\gamma_s > 1$. The easiest slip system for this geometry is on the $(1\bar{1}1)$ plane, along the [121] direction, with corresponding angles $\theta = 54.7^0$ and $\phi = 60^0$. We find that for this geometry, $G_d/2\gamma_s = 1.74$, a value which indicates that dislocation emission is energetically unfavorable compared to crack propagation by cleavage, since according to the Griffith criterion [Griffith (1920)] the critical loading for cleavage is $G_c = 2\gamma_s$. This result then implies that all cracks on (001) planes are brittle and that (001) planes in aluminum are intrinsically cleavable. In light of experimental evidence that suggests aluminum to be ductile, this is a surprising result. We return to this point below.

A different way to link the present results to the intrinsic brittleness or ductility of aluminum, is through comparison to recent atomistic calculations on model systems. The work of Zhou et al. (1993,1994) has investigated the conditions for ductile vs. brittle behavior in a model material, which consisted of a two-dimensional solid of atoms interacting through a variety of empirical potentials. These authors find that the ratio $\gamma_{us}^{(r)}/\mu b$ provides a useful means for characterizing the D/B behavior, with the value 0.015 separating the two regimes, and ductile behavior corresponding to smaller values of the ratio. From the results of the present study, we find that

$$\frac{\gamma_{us}^{(r)}}{\mu b} = 0.0287 \tag{10}$$

when we use the value of μ calculated at the theoretical lattice constant of 3.95 Å. Our value for the ratio that characterizes D/B behavior is larger than the criterion of Zhou et al. (1993,1994) by almost a factor of 2, again implying a brittle behavior for aluminum within this theoretical model.

One may question the ability of the present calculations to obtain accurate estimates of the fundamental quantities entering the D/B criteria. In defense of the accuracy of the present calculations (putting aside the careful comparison of theoretical results to available experimental numbers discussed in Section II), we invoke the following argument: Suppose that experimental numbers were used exclusively for the values of key quantities. A strict lower bound for the value of γ_{us} is the value of γ_{isf}, since the unstable stacking energy cannot be lower than the energy of the instrinsic stacking fault. Using the value of γ_{isf} as an approximation to γ_{us} and the experimental values for $\mu = 26.5$ GPa and $b = a_0/\sqrt{6}$, $a_0 = 4.05$ Å, one would obtain a ratio of $\gamma_{us}/\mu b$ in the range of 0.025 to 0.064 (from the experimental values for γ_{isf} which range

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from 0.11 to 0.28 J/m^2). This is a lower bound (since γ_{isf} is a lower bound for γ_{us}) and is still much higher than the value of 0.015 proposed by Zhou et al. (1993,1994) as separating brittle from ductile behavior. In fact, the lowest value of this estimate is reasonably close to the result obtained from our first-principles calculations. This argument leads us to suggest that the surprising result obtained here, namely that aluminum is predicted to be brittle, is not due to limitations of the first-principles calculations.

We also wish to point out that surface energy terms associated with surface creation during dislocation emission and lattice trapping were not taken into account in the Peierls type analysis discussed above. Both of these effects would tend to *increase* the value of the ratio $G_d/2\gamma_s$ relative to what has been reported here [see for example, Xu, Argon and Ortiz (1995); Juan, Kaxiras and Sun (1996)], titling the balance toward more brittle behavior. On the other hand, the atomistic simulations of Zhou et al. (1993,1994) which do take these effects into account, they nevertheless provide a picture consistent with the Peierls analysis.

These results pose an interesting puzzle. To our knowledge, there is no experimental indication of brittle behavior in aluminum at finite temperature. The resolution of the puzzle may be provided by three different possibilities: (a) The theoretical framework invoked to discuss D/B behavior applies to the *intrinsic* behavior of a pure material; the behavior of a material with high density of pre-existing dislocations is not captured by this framework. Thus, aluminum may be ductile due to motion of pre-existing dislocations. Beltz, Rice, Shih and Xia (1996) recently addressed the issue of crack growth in the presence of a large number of pre-existing dislocations. Their analysis could provide important insight to the problem discussed here. (b) Since, strictly speaking, the theoretical analysis presented above applies to zero temperature, aluminum may indeed be brittle at zero temperature and its ductility is due to thermally activated dislocation emission. Rice and Beltz (1994) have extended the Peierls framework to study thermally activated dislocation emission in certain cases. (c) Finally, it is possible that significant improvements are required in order to provide quantitative theories that can predict the intrinsic D/B behavior of a pure material. For example, the recent results of Xu, Argon and Ortiz (1996b) point to exciting new directions toward developing quantitative theories of the D/B transition that include more realistic representation of dislocation nucleation processes near a crack tip.

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TABLE I

	a_0 (Å)	B	C_{44}	$C_{11} - C_{12}$	μ
Experiment	4.05	76.9	28.5	46.9	26.5
Present work (at T = 0 K)	3.95 (−2%)	84.8 (+10%)	45.5 (+60%)	58.8 (+25%)	39.1 (+48%)
Present work at $a_0' = 4.05$ Å			29.7 (+4%)	45.1 (−4%)	26.8 (+1%)
Mehl and Boyer (1991) at $a_0' = 4.05$ Å			28.5 (0%)	50.0 (+7%)	27.1 (+2%)

TABLE I: Comparison of experimental and theoretical values for the lattice constant a_0, bulk modulus B, elastic constants $C_{44}, C_{11} - C_{12}$, and shear modulus μ, evaluated at the theoretical zero-temperature equilibrium value of the lattice constant (3.95 Å) and the room-temperature experimental one (4.05 Å). Elastic constants and moduli are given in units of GPa and the experimental values are taken from Hirth and Lothe (1982). The numbers in parentheses give the percent difference between theoretical and experimental values.

TABLE II

	$\gamma_{us}^{(u)}$ (J/m²)	$\gamma_{us}^{(r)}$ (J/m²)	γ_s (J/m²)	$b/2(a_0/\sqrt{6})$	L/b	$p = \Delta\theta^*/L$	$q = \gamma_{us}^{(u)}/2\gamma_s$
DFT/LDA	0.244	0.224	1.10	0.62	0.135	0.111	0.287
EAM	0.092	0.079	0.57	0.50	0.140	0.0854	0.279

TABLE II: The values of the unstable stacking energy for unrelaxed $\gamma_{us}^{(u)}$ and relaxed $\gamma_{us}^{(r)}$ configurations, the surface energy γ_s, the displacement $b/2$ corresponding to the unstable stacking energy along the slip route (in units of the intrinsic stacking fault slip $a_0/\sqrt{6}$), the length scale L for tension, and the scaled parameters p, q that determine tension to shear coupling [see text and Sun, Beltz and Rice (1993)]. The DFT/LDA values are from the present calculation, the EAM values from the work of Sun et al. (1993). The DFT/LDA value of γ_s is from Ferrante and Smith (1979).

TABLE III

Configuration	$\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$	Slip system	(θ, ϕ)	$G_d/(2\gamma_s)$
A	$\{[\bar{1}10],[001],[110]\}$	$\frac{1}{6}[121](1\bar{1}1)$	$(54.7^0, 60^0)$	1.740
B	$\{[001],[\bar{1}10],[110]\}$	$\frac{1}{6}[\bar{1}12](\bar{1}1\bar{1})$	$(35.3^0, 0^0)$	0.968
C	$\{[111], [1\bar{1}0], [11\bar{2}]\}$	$\frac{1}{6}[2\bar{1}\bar{1}](11\bar{1})$	$(90^0, 30^0)$	0.730
D	$\{[1\bar{1}2], [\bar{1}11], [110]\}$	$\frac{1}{6}[\bar{1}12](\bar{1}1\bar{1})$	$(70.5^0, 0^0)$	0.504

TABLE III: Ratio of the critical loading for dislocation emission G_d to cleavage energy $(2\gamma_s)$, as obtained form the Peierls model analysis, for various configurations of the slip plane and the emited dislocation, characterized by the three vectors $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$ and the angles (θ, ϕ) (see text and Fig. 4). A ratio greater than 1 indicates brittle failure, as in configuration A.

FIG. 1: Illustration of the atomic arrangement in fcc aluminum and the slab configuration used in the calculations. Atoms in the three layers of stacking along the [111] crystallographic direction are marked by different symbols. (a) Top view, (b) side view, indicating the plane on which the crystal is sheared.

FIG. 2: Convergence tests for the value of the intrinsic stacking fault energy of aluminum, as a function of plane wave basis size at fixed number of sampling points (top panel) and as a function of number of sampling points in the Brillouin Zone at fixed plane-wave basis size N_{PW} (bottom panel). Calculations for slabs of two different sizes containing 6 and 9 layers along the [111] direction are shown, as well as those from the ANNNI model (see text for details).

FIG. 3: Generlaized stacking fault energy γ_{gsf} as a function of displacement along the slip route in aluminum. Points are calculated values, the line is a polynomial fit. The maximum in the energy corresponds to the unstable stacking energy γ_{us}, before atomic and volume relaxation. The end point corresponds to the instrinsic stacking fault energy γ_{isf}. Note that the maximum occurs slightly to the right of the middle.

FIG. 4: Schematic representation of the geometry for dislocation emmision from the crack tip. The vectors $\{\vec{a}_1, \vec{a}_2, \vec{a}_3\}$ are along the extension of the crack, perpendicular to the crack plane and along the crack line, respectively. θ is the angle between the crack plane and the inclined plane on which the dilsocation with Burgers vector b is emmited, and ϕ is the angle between the emmision direction and the Burgers vector.